Package 'PUPAIM'

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Type Package

Title A Collection of Physical and Chemical Adsorption Isotherm Models

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Description Adsorption isotherm equations are linearized plots of different solid-liquid phase equilibria used in calculating different parameters related to the adsorption process. Isotherm equations deals with physical adsorption of gases and vapor and gives the most important characteristics of industrial adsorbents that include pore volume, pore size or energy distribution. PUPAIM has 28 documented adsorption isotherm models listed by Dabrowski (2001) <doi:10.1016/S0001-8686(00)00082-8> and Ayawei et al.(2017) <doi:10.1155/2017/3039817>. These models could be easily fitted in R using adsorption data (Ce and Qe) obtained from experiments.

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R topics documented:

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banana *Banana Adsorption Study*

Description

Actual adosrption experiment results using Musa paradisiaca peels.

Usage

```
banana
```

Format

A data frame with 6 observations on the following 2 variables.

`Ce` a numeric vector

`Qe` a numeric vector

...

`bauduanalysis` *Baudu Isotherm Analysis Non-Linear Form*

Description

Baudu is a reduced form of the Langmuir Isotherm upon observation that the estimation of Langmuir coefficients, b and q, by measurement of tangents at different equilibrium concentrations shows that they are not constants in a broad range.

Usage

```
bauduanalysis(Ce, Qe)
```

Arguments

`Ce`	the numerical value for the equilibrium capacity
`Qe`	the numericl value for the adsorbed capacity

Value

the nonlinear regression and the parameters for the Baudu isotherm

Author(s)

Roan Maeve E.Arilla

Daren Mae B. Imperial

C.C. Deocaris

References

Ayawei, N., Ebelegi, A. and Wankasi, D. (2017). Modelling and Interpretation of Adsorption Isotherms. Journal of Chemistry, 2017, pp.1-12. doi: 10.1155/2017/3039817

Subramania, D. and Ramadoss, R. (2018). Adsorption of Chromium Using Blue Green Algae-Modeling and Application of Various Isotherms. International Journal of Chemical Technology, 10(1), pp.1-22.

Examples

```
bauduanalysis(c(.014, .063, .094, .2, .385, 1.15, 1.64), c(.072, .213, .282, .32, .325, .338, .344))
```

bauduplot *Baudu Isotherm Plot*

Description

Plot of the analysis of Baudu Isotherm

Usage

```
bauduplot(Ce, Qe)
```

Arguments

Ce	the numerical value for the equilibrium capacity
Qe	the numerical value for the adsorbed capacity

Value

the LSRL plot of Baudu isotherm analysis @export

BETanalysis *BET Isotherm Analysis Non-Linear Form*

Description

An isotherm that takes account of the possibility that the monolayer in the Langmuir adsorption isotherm can act as a substrate for further adsorption.

Usage

```
BETanalysis(Ce, Qe)
```

Arguments

Ce	the numerical value for the equilibrium capacity
Qe	the numerical value for the adsorbed capacity

Value

the non-linear regression, errors, and the parameter values for the BET Isotherm Model

Author(s)

Geraldine N. Aliman

Cherry Rose E. Olivar

C.C. Deocaris

References

Shipu, S.(2014, April 30). Bet Isotherm. Retrived form https://www.slideshare.net/mobile/Sourav44Shipu/bet-isotherm

Examples

```
BETanalysis(c(.014, .063, .094, .2, .385, 1.15, 1.64), c(.072, .213, .282, .32, .325, .338, .344))
```

`deltaG` *Gibbs free energy of Adsorption*

Description

Defines the spontaneity of an adsoprtion process base from the value. If it is negative is is spontaneous and if the result is positive,the reaction is not spontaneous.

Usage

```
deltaG(t, K)
```

Arguments

`t`	temperature used in the experiment
`K`	equilirium constant for the adsorption process

Value

the Gibbs free energy value for the given adsorption process in terms of Kj(kilojoule) per mole

Examples

```
deltaG(25,1234)
```

`dubininradanalysis` *Dubinin-Radushkevich Isotherm Analysis Non-Linear Form*

Description

It is an empirical generally applied to express adsorption mechanism with Gaussian energy distribution onto heterogeneous surfaces (Tsamo, et,al, 2019). In the non-linear form, qe =Xm*exp(-K*Ce^2). The said model has often fitted high solute activities and the intermediate range of concentrations as well. One unique feature of the said model is that it is temperature-dependent (Dada, et, al, 2012).

Usage

```
dubininradanalysis(Ce, Qe)
```

Arguments

Ce	the numerical value for the equilibrium capacity
Qe	the numerical value for the adsorbed capacity

Value

the linear regression, errors, and the parameter values (Xm, and K) for the Dubinin-Radushkevich Isotherm Model

Author(s)

Morales, Dale Jonathan, M.

C.C. Deocaris

References

One-, Two-, and Three-Parameter Isotherms, Kinetics, and Thermodynamic Evaluation of Co(II) Removal from Aqueous Solution Using Dead Neem Leaves, Tsamo, et,al. (2019), Volume 2019, https://doi.org/10.1155/2019/6452672

Langmuir, Freundlich, Temkin, and Dubinin-Radushkevich Isotherms Studies of Equilibrium Sorption of Zn^+2 Unto Phosphoric Acid Modified Rise Husk, Dada, et, al, (2012), Journal of Applied Chemistry, Volume 3, Issue 1, pp 38-45, www.iosrjournals.org

Examples

```
Ce <- c(0.01353, 0.04648, 0.13239, 0.27714, 0.41600, 0.63607, 0.80435, 1.10327, 1.58223)
Qe <- c(0.03409, 0.06025, 0.10622, 0.12842, 0.15299, 0.15379, 0.15735, 0.15735, 0.16607)
dubininradanalysis(Ce, Qe)
```

---

elovichanalysis *Elovich Isotherm Analysis Non-Linear Form*

Description

Elovich empirical adsorption model is based on the assumption of energetic heterogeneity of the adsorption sites. Moreover, elovich maximum adsorption capacity and Elovich constant can be calculated from the slopes and the intercepts of the plot ln(Qe/Ce) versus Qe.

Usage

```
elovichanalysis(Qe, Ce)
```

Arguments

Qe	the numerical value for adsorbed capacity
Ce	the numerical value for equilibrium concentration

Value

the linear regression and the parameters for the Elovich isotherm

Author(s)

Edmundo B. De Guzman Jr.

C.C. Deocaris

References

Ayawei, N., Ebelegi, A.N., & Wankasi, D. (2017). Modelling and Interpretation of Adsorption Isotherms. Journal of Chemistry, 2017, 1-11. doi: 10.1155/2017/3039817

Gutierrez, L.G., Moreno-Pirajan, J.C., Guarin Romero, J.R. (2018). Kinetic and Equilibrium Study of the Adsorption of CO2 in Ultramicropores of Resorcinol-Formaldehyde Aerogels Obtained in Acidic and Basic Medium. Journal of Carbon Research, 2018, pp. 4. doi:10.3390/c4040052

Farouq, R., & Yousef, N.S. (2015). Equilibrium and Kinetics Studies of Adsorption of Copper(II) Ions on Natural Biosorbent. International Journal of Chemical Engineering and Applications, 2015, pp.332. DOI: 10.7763/IJCEA.2015.V6.503

Examples

```
Ce <- c(0.01353, 0.04648, 0.13239, 0.27714, 0.41600, 0.63607, 0.80435, 1.10327, 1.58223)
Qe <- c(0.03409, 0.06025, 0.10622, 0.12842, 0.15299, 0.15379, 0.15735, 0.15735, 0.16607)
elovichanalysis(Qe, Ce)
```

---

elovichkinetics *Elovich Kinetics*

Description

This equation assumes that the actual solid surfaces are energetically heterogenous and that neither desorption nor interactions betwen adsorbed species could subcutaneously affect the kinetics of adsorption at low surface coverage. (Mercado-Borayo, et. al, 2014)

Usage

```
elovichkinetics(t, Qt)
```

Arguments

t	duration for the experiment
Qt	the numerical value for the concentration at given time

Value

The regression analysis for the Elovich Kinetics

`fhanalysis` *Flory-Huggins Isotherm Analysis Non-Linear Form*

Description

Flory-Huggins isotherm is a two-parameter isotherm that describes the degree of surface coverage characteristics of the adsorbate on the adsorbent. This isotherm model can express the feasibility and spontaneity of an adsorption process.

Usage

```
fhanalysis(Ce, Qe)
```

Arguments

`Ce`	is equal to Co which is the numeric value for the iniztial concentration
`Qe`	is equal to theta which is the degree of surface coverage

Value

the nonlinear regression and the parameters for the Flory-Huggins isotherm

Author(s)

Carmela L. Barbacena

C.C. Deocaris

References

Ayawei, N., et al., (5 September 2017). Modeling and Interpretation of Adsorption Isotherms. Retrieved from: https:// www.hindawi.com/journals/jchem/2017/3039817/

Tsamo, C., et al., (27 November 2019). One-, Two-, and Three- Parameter Isotherms, Kinetics, and Thermodynamic Evaluation of Co

Examples

```
Ce <- c(0.01353, 0.04648, 0.13239, 0.27714, 0.41600, 0.63607, 0.80435, 1.10327, 1.58223)
Qe <- c(0.03409, 0.06025, 0.10622, 0.12842, 0.15299, 0.15379, 0.15735, 0.15735, 0.16607)
fhanalysis(Ce, Qe)
```

firstorder *Pseudo-1st Order Kinetics*

Description

A first-order rate equation which is believed to be the earliest model that was presented by Lagergen (1898) to describe the kinetic process of liqud-solid phase adsorption of oxalic acid and malonic acid onto charcoal pertains to the adsorption rate based on the adsorption capacity.

Usage

```
firstorder(t, Ce)
```

Arguments

t	duration of the experiment
Ce	the numerical value for the equilibrium capacity

Value

the regression analysis for the first order kinetics

Examples

```
firstorder(c(1,2,3,4,5),c(1,2,3,4,5))
```

fiveparamanalysis *Five Parameter Isotherm Analysis*

Description

A five-parameter empirical model that is capable of simulating the model variations that applies over a wide range of equilibrium data. Its increased parameters provides a more accurate non linear regression, better than two, three or four parameters. (Subramanyam and Ashutosh, 2009)

Usage

```
fiveparamanalysis(Ce, Qe)
```

Arguments

Ce	the numerical value for the equilibrium capacity
Qe	the numerical value for the adsorbed capacity

Value

the non linear regression and the parameters for the five parameter non-linear isotherm analysis

Author(s)

Jeff Ryan S. Magalong

Joshua Dela Cruz

Chester C. Deocaris

References

Fritz, W., & Schluender, E.U. (1974). Simultaneous adsorption equilibria of organic solutes in dilute aqueous solutions on activated carbon. Chemical Engineering Science, 29(5), 1279-1282. <doi: 10.1016/0009-2509(74)80128-4>

@references Subramanyam, B., & Das, A. (2009). Study of the adsorption of phenol by two soils based on kinetic and isotherm modeling analyses. Desalination, 249(3), 914-921. <doi:10.1016/j.desal.2009.05.020>

Examples

```
Ce <- c(0.01353, 0.04648, 0.13239, 0.27714, 0.41600, 0.63607, 0.80435, 1.10327, 1.58223)
Qe <- c(0.03409, 0.06025, 0.10622, 0.12842, 0.15299, 0.15379, 0.15735, 0.15735, 0.16607)
fiveparamanalysis(Ce, Qe)
```

---

fowlerganalysis *Fowler-Guggenheim Isotherm Analysis Non-Linear Form*

Description

Fowler-Guggenheim isotherm model describes as a case where there is mobile adsorption as well as lateral interaction among molecules.

Usage

```
fowlerganalysis(theta, Ce, t)
```

Arguments

theta	the numerical value for the surface coverage/fractional coverage
Ce	the numerical value for the equilibrium capacity
t	the numerical value for temperature in Kelvin

Author(s)

William Peter G. Sarmiento

Chester C. Deocaris

References

Ayawei, N., Ebelegi, A.N., & Wankasi, D. (2017). Modelling and Interpretation of Adsorption Isotherms. Journal of Chemistry, 2017, 1-11. doi: 10.1155/2017/3039817

Qing Shao and Carol K Hall (2016). Protein adsorption on nanoparticles: model development using computer simulation. Journal of Physics: Condensed Matter

Oualid Hamdaouia, Emmanuel Naffrechoux (2007). Modeling of adsorption isotherms of phenol andchlorophenols onto granular activated carbonPart I. Two-parameter models and equations allowing determination of thermodynamic parameters

Examples

```
Ce <- c(0.39, 0.74, 1.19, 1.63, 2.03, 2.51, 2.96, 3.46, 3.9, 4.35)
theta <- c(0.051, 0.12, 0.14, 0.17, 0.21, 0.22, 0.24, 0.24, 0.27, 0.29)
fowlerganalysis(theta, Ce, 298)
```

---

fractionalpower *Fractional Power Kinetic Model*

Description

Calculates Kt parameter of the Fractional power kinetic model.

Usage

```
fractionalpower(t, qt)
```

Arguments

t	duration of the experiment
qt	the numerical value for the equilibrium capacity

Value

the regression analysis for the first order kinetics

Examples

```
fractionalpower (c(1,2,3,4,5),c(1,2,3,4,5))
```

`freundlich.LM` *Freundlich Isotherm Analysis Linear Form*

Description

This isotherm model predicts the logarithmic relationship of equilibrium capacity and adsorbed capacity (Gessner and Hasan, 1987). Furthermore, this model gives an equation which defines the surface heterogeneity and the exponential distribution of active sites (Ayawei, et al., 2017).

Usage

```
freundlich.LM(Ce, Qe)
```

Arguments

`Ce`	the numerical value for the equilibrium capacity
`Qe`	the numerical value for the adsorbed capacity

Value

the linear regression and the parameters for the Freundlich isotherm

Author(s)

Carl Luis P. Flestado

Chester C. Deocaris

References

Ayawei, N., Ebelegi, A. N., & Wankasi, D. (2017). Modelling and Interpretation of Adsorption Isotherms. Journal of Chemistry, 2017, 1–11. doi: 10.1155/2017/3039817

Gessner, P. K., & Hasan, M. M. (1987). Freundlich and Langmuir Isotherms as Models for the Adsorption of Toxicants on Activated Charcoal. Journal of Pharmaceutical Sciences, 76(4), 319–327. doi: 10.1002/jps.2600760412

Examples

```
Ce <- c(0.01353, 0.04648, 0.13239, 0.27714, 0.41600, 0.63607, 0.80435, 1.10327, 1.58223)
Qe <- c(0.03409, 0.06025, 0.10622, 0.12842, 0.15299, 0.15379, 0.15735, 0.15735, 0.16607)
freundlich.LM (Ce, Qe)
```

`freundlichanalysis` *Freundlich Isotherm Analysis Non-Linear Form*

Description

This isotherm model is an empirical model applicable to diluted solutions adsorption processes (Gessner and Hasan, 1987). Furthermore, this model gives an equation which defines the surface heterogeneity and the exponential distribution of active sites (Ayawei, et al., 2017).

Usage

```
freundlichanalysis(Ce, Qe)
```

Arguments

`Ce`	the numerical value for the equilibrium capacity
`Qe`	the numerical value for the adsorbed capacity

Value

the nonlinear regression and the parameters for the Freundlich isotherm

Author(s)

Carl Luis P. Flestado

C.C. Deocaris

References

Ayawei, N., Ebelegi, A. N., & Wankasi, D. (2017). Modelling and Interpretation of Adsorption Isotherms. Journal of Chemistry, 2017, 1–11. doi: 10.1155/2017/3039817

Gessner, P. K., & Hasan, M. M. (1987). Freundlich and Langmuir Isotherms as Models for the Adsorption of Toxicants on Activated Charcoal. Journal of Pharmaceutical Sciences, 76(4), 319–327. doi: 10.1002/jps.2600760412

Examples

```
Ce <- c(0.01353, 0.04648, 0.13239, 0.27714, 0.41600, 0.63607, 0.80435, 1.10327, 1.58223)
Qe <- c(0.03409, 0.06025, 0.10622, 0.12842, 0.15299, 0.15379, 0.15735, 0.15735, 0.16607)
```

`fritzanalysis` *Fritz-Schluender Isotherm Analysis Non-Linear Form*

Description

An empirical equation which can fit a wide range of experimental results because of the large number of coefficients in the isotherm.

Usage

```
fritzanalysis(Ce, Qe)
```

Arguments

`Ce`	the numerical value for the equilibrium capacity
`Qe`	the numerical value for the adsorbed capacity

Value

the nonlinear regression and the parameters for the Fritz-Schlunder isotherm

Author(s)

Diego Calamba

Rain Grace R. Reyes

C.C. Deocaris

References

Aljeboree, A. M., Alshirifi, A. N., & Alkaim, A. F. (2017). Kinetics and equilibrium study for the adsorption of textile dyes on coconut shell activated carbon. Arabian Journal of Chemistry, 10, S3381-S3393. doi: 10.1016/j.arabjc.2014.01.020

Examples

```
fritzanalysis(moringa$Ce, moringa$Qe)
```

halseyanalysis *Halsey Isotherm Analysis Non-Linear Form*

Description

used to evaluate multilayer adsorption at a relatively large distance from the surface

Usage

```
halseyanalysis(Ce, Qe)
```

Arguments

Ce	the numerical value for the equilibrium capacity
Qe	the numerical value for the adsorbed capacity

Value

the nonlinear regression and the parameters for the Halsey isotherm analysis

Author(s)

Aries N. Bunag

C.C. Deocaris

References

Sousa Neto, V.O., Oliveira, A. G., Teixeira, R.N.P., Silva, M.A.A.,Freire, P.T.C., Keukeleire, D.D., & Nascimento, R.S.(2011). USE OF COCONUT BAGASSE AS ALTERNATIVE ADSORBENT FOR SEPARATION OF COPPER(III) IONS FROM AQUEOUS SOLUTIONS: ISOTHERMS, KINETIC AND THERMODYNAMIC STUDIES. Retrived February 17, 2020, from https://bioresources.cnr.ncsu.edu/BioRes_

Imran, M., Naseem, Khalida, Mirza, Latif, M., & Madeeha. (2018, December 1). Evaluation of Saccharum bengalense as a Non-Conventional Biomaterial for Biosorption of Mn(II) Ions from Aqueous Solutions. Retrieved February 17.2020, from http://www.ijcce.ac.ir/article_29361.html

Examples

```
Ce <- c(0.01353, 0.04648, 0.13239, 0.27714, 0.41600, 0.63607, 0.80435, 1.10327, 1.58223)
Qe <- c(0.03409, 0.06025, 0.10622, 0.12842, 0.15299, 0.15379, 0.15735, 0.15735, 0.16607)
halseyanalysis(Ce, Qe)
```

`harkinsjuraanalysis` *HarkinsJura Isotherm Analysis Non-Linear Form*

Description

It assumes the possibility of multilayer adsorption on the surface of absorbents having heterogenous pore distribution (Ayawei, et al., 2017),(Gupta, et al., 2012)

Usage

```
harkinsjuraanalysis(Ce, Qe)
```

Arguments

`Ce`	the numerical value for the equilibrium capacity
`Qe`	the numerical value for the adsorbed capacity

Value

the nonlinear regression and the parameters for the HarkinsJura isotherm

Author(s)

Raymond James L. Adame

C.C. Deocaris

References

Ayawei, N., Ebelegi, A. N., & Wankasi, D. (2017). Modelling and Interpretation of Adsorption Isotherms. Journal of Chemistry, 2017, 1-11. doi: 10.1155/2017/3039817

Gupta, V. K., Pathania, D., Agarwal, S., & Sharma, S. (2012). Removal of Cr(VI) onto Ficus carica biosorbent from water. Environmental Science and Pollution Research, 20(4), 2632-2644. doi:10.1007/s11356-012-1176-6

Examples

```
Ce <- c(0.01353, 0.04648, 0.13239, 0.27714, 0.41600, 0.63607, 0.80435, 1.10327, 1.58223)
Qe <- c(0.03409, 0.06025, 0.10622, 0.12842, 0.15299, 0.15379, 0.15735, 0.15735, 0.16607)
harkinsjuraanalysis(Ce, Qe)
```

henryanalysis *Henry's Isotherm*

Description

It describes the appropriate fit to the adsorption of adsorbate at relatively low concentrations such that all adsorbate molecules are secluded from their nearest neighbours.

Usage

```
henryanalysis(Ce, Qe)
```

Arguments

Ce	the numerical value for the equilibrium capacity
Qe	the numerical value for the adsorbed capacity

Value

the linear regression and the parameter for the henry isotherm analysis

Author(s)

De Osio, Lloyd P.

References

Ayawei, N., Ebelegi, A. N., and Wankasi, D. (2017). Review Article: Modelling and interpretation of Adsorption isotherms. HINDAWI: Journal of Chemistry. doi: 10.1155/2017/3039817

Bayuo, J. Pelig-Ba, K.B., and Abukari, M.A. (2018). Isotherm modelling of lead (II) adsorption from aqueous solution using groundnut shell as a low-cost adsorbent. IOSR Journal of Appplied chemistry doi:10.9790/5736-1111011823

Examples

```
Ce <- c(0.01353, 0.04648, 0.13239, 0.27714, 0.41600, 0.63607, 0.80435, 1.10327, 1.58223)
Qe <- c(0.03409, 0.06025, 0.10622, 0.12842, 0.15299, 0.15379, 0.15735, 0.15735, 0.16607)
henryanalysis (Ce, Qe)
```

`hillanalysis` *Hill Isotherm Analysis Non-Linear Form*

Description

Hill isotherm model shows the connection of different species of homogeneous surfaces. It assumes that the adsorption is a cooperative phenomenon, with a ligand binding activity at one part of a macromolecule that may affect the different binding sites of that same macromolecule.

Usage

```
hillanalysis(Ce, Qe)
```

Arguments

`Ce`	equilibrium capacity
`Qe`	adsorbed capacity

Author(s)

Amiela D. Suerte

Carl Luis P. Flestado

C.C. Deocaris

References

Tanzifi, M., Karimipour, K., Hoseini, S., Ali, I.(2017). Artificial neural network optimization for methyl orange adsorption onto polyaniline nano-adsorbent: Kinetic, isotherms and thermodynamics. Journal of Molecular Liquids, 2017, p.11. DOI:10.1016/j.molliq.2017.08.122

Saadi, R., Saadi, z., Fazaeli, R., Fard, N.E.(2015). Monolayer and multilayer adsorption models for sorption aqueous media. Korean Journal of Chemical Engineering, 2015, p.5. DOI: 10.007/s11814-015-0053-7

Larimi, S.G., Moghadamnia, A.A., Najafpour, G.(2016). Kinetics and isotherm studies of the Immobilized Lipase on Chitosan Support. International Journal of Engineering, 2026, p.12. DOI: 10.5829/idosi.ije.2016.29.10a.01

Examples

```
Ce <- c(0.001, 0.0026, 0.0125, 0.031, 0.056)
Qe <- c(0.02, 0.072, 0.146, 0.15, 0.151)
hillanalysis(Ce, Qe)
```

`hilldeboeranalysis` *Hill-Deboer Isotherm Non-linear Analysis*

Description

Hill-Deboer isotherm model describes as a case where there is mobile adsorption as well as lateral interaction among molecules.

Usage

```
hilldeboeranalysis(theta, Ce, t)
```

Arguments

`theta`	the numerical value for the surface converage / fractional coverage
`Ce`	the numerical value for the equilibrium capacity
`t`	the numerical value for the temperature of the adsorption experimentation in Kelvin

Author(s)

Benz L. Rivera

Jeff Ryan S. Magalong

C.C. Deocaris

References

Ayawei, N., Ebelegi, A.N., & Wankasi, D. (2017). Modelling and Interpretation of Adsorption Isotherms. Journal of Chemistry, 2017, 1-11. doi 10.115520173039817

Qing Shao and Carol K Hall (2016). Protein adsorption on nanoparticles model development using computer simulation. Journal of Physics Condensed Matter

Oualid Hamdaouia, Emmanuel Naffrechoux (2007). Modeling of adsorption isotherms of phenol andchlorophenols onto granular activated carbonPart I. Two-parameter models and equations allowing determination of thermodynamic parameters

Examples

```
Ce <- c(0.39, 0.74, 1.19, 1.63, 2.03, 2.51, 2.96, 3.46, 3.9, 4.35)
theta <- c(0.051, 0.12, 0.14, 0.17, 0.21, 0.22, 0.24, 0.24, 0.27, 0.29)
hilldeboeranalysis(theta, Ce, 298)
```

`jossensanalysis` *Jossens Isotherm Analysis Non-Linear Form*

Description

The Jossens isotherm model predicts a simple equation based on the energy distribution of adsorbate-adsorbent interactions at adsorption sites. This model assumes that the adsorbent has heterogeneous surface with respect to the interactions it has with the adsorbate.

Usage

```
jossensanalysis(Qe, Ce)
```

Arguments

`Qe`	the numerical value for the adsorbed capacity
`Ce`	the numerical value for the equilibrium capacity

Value

the nonlinear regression and the parameters for the Jossens isotherm

Author(s)

Stephanie Mae L. Manuel

Marie Aileen M. Allauigan

C.C. Deocaris

References

Ayawei, N., Ebelegi, A., & Wankasi, D. (2017, September 5). Modelling and Interpretation of Adsorption Isotherms. Journal of Chemistry, 2017, 6. doi:10.1155/2017/3039817

Examples

```
jossensanalysis(c(1,2,3,4,5),c(1,2,3,4,5))
```

`jovanovicanalysis` *Jovanovic Isotherm Analysis Non-Linear Form*

Description

It is predicated on the assumptions contained in the Langmuir model, but in addition the possibility of some mechanical contacts between the adsorbate and adsorbent

Usage

```
jovanovicanalysis(Ce, Qe)
```

Arguments

`Ce`	the numerical value for the equilibrium capacity
`Qe`	the numerical value for the adsorpted capacity

Value

the nonlinear regression and the parameters for the Jovanovic isotherm

Author(s)

Christian Josuah F. Maylas

C.C. Deocaris

References

: Saadi, R., Saadi, Z., Fazaeli, R., Fard, N. E. (2015). Monolayer and multilayer adsorption isotherm models for sorption from aqueous media. Korean J. Chem. Eng., 32(5), 787-799 (2015) DOI: 10.1007/s11814-015-0053-7

: Vargas, A., Cazetta, A., Kunita, M., Silva, T., Almeida V. (2011). Adsorption of methylene blue on activated carbon produced from ?amboyant pods (Delonix regia): Study of adsorption isotherms and kinetic models. Chemical Engineering Journal 168 (2011) 722-730

Examples

```
jovanovicanalysis(moringa$Ce, moringa$Qe)
```

kahnanalysis *Kahn Isotherm Analysis Non-Linear Form*

Description

Kahn isotherm model is a general model for adsorption of biadsorbate from pure dilute equations solutions

Usage

```
kahnanalysis(Ce, Qe)
```

Arguments

Ce	the numerical value for the equilibrium capacity
Qe	the numerical value the absorbed capacity

Value

the linear regression and the parameters for the Kahn isotherm analysis

Author(s)

Jann Audrey B. Angeles

Raymond B. Diaz

C.C. Deocaris

References

A. R. Khan, R. Ataullah,A. Al-Haddad. (1997). Equilibrium Adsorption Studies of Some Aromatic Pollutants from Dilute Aqueous Solutions on Activated Carbonat Different Temperatures. JOURNAL OF COLLOID AND INTERFACE SCIENCE, 154-165.

Tosun, I. (2012). Ammonium Removal from Aqueous Solutions by Clinoptilolite: Determination of Isotherm and Thermodynamic Parameters and Comparison of Kinetics by the Double Exponential Model and Conventional Kinetic Models. International Journal of Environmental Research and Public Health , 970-984.

Examples

```
kahnanalysis(c(0.5, 0.6, 0.7, 1.3, 3.9, 7.6, 16.5),c(4.5, 6.5, 9.3, 10.7, 11.6, 12.5, 13.7))
```

kiselevanalysis *Kiselev Isotherm Non linear Analysis*

Description

It is also known as localized monomolecular layer model and is only valid for surface coverage theta > 0.68.

Usage

```
kiselevanalysis(theta, Ce)
```

Arguments

theta	the numerical value for surface coverage
Ce	the numerical value for equilibrium capacity

Value

the linear regression and the parameters for the Kiselev isotherm analysis

Author(s)

Ashley Quebrado

C. C. Deocaris

Examples

```
Ce <- c(0.01353, 0.04648, 0.13239, 0.27714, 0.41600, 0.63607, 0.80435, 1.10327, 1.58223)
Qe <- c(0.03409, 0.06025, 0.10622, 0.12842, 0.15299, 0.15379, 0.15735, 0.15735, 0.16607)
kiselevanalysis(Ce, Qe)
```

koblecarrigananalysis *Koble-Carrigan Isotherm*

Description

It is three-parameter isotherm model equation that incorporates both Freundlich and Langmuir isotherms for representing equilibrium adsorption data. Koble-Corrigan isotherm model appeared to have advantages over both the Langmuir and Freundlich equations in that it expresses adsorption data over very wide ranges of pressures and temperatures.

Usage

```
koblecarrigananalysis(Ce, Qe)
```

Arguments

Ce	the numerical value for the equilibrium capacity
Qe	the numerical value for the adsorbed capacity

Value

the nonlinear regression and the parameters for the Koble-Carrigan isotherm analysis

Author(s)

Reinald L. Claudio

Verna Chin DR. Caparanga

C.C. Deocaris

References

Ayawei, N., Ebelegi, A. N., & Wankasi, D. (2017). Modelling and Interpretation of Adsorption Isotherms. Journal of Chemistry, 2017, 1-11. doi: 10.1155/2017/3039817

Koble, R., & Corrigan, T., "Adsorption isotherms for pure hydrocarbons," Industrial and Engineering Chemistry, vol. 44, no. 2, pp. 383-387, 1952.

Examples

```
koblecarrigananalysis(moringa$Ce, moringa$Qe)
```

---

langmuir.LM1 *Langmuir Isotherm Analysis Linear Form*

Description

The Langmuir Linear Equation I adsorption isotherm is used to describe the equilibrium between adsorbate and adsorbent system, where the adsorbate adsorption is limited to one molecular layer at or before a relative pressure of unity is reached.

Usage

```
langmuir.LM1(Ce, Qe)
```

Arguments

Ce	the numerical value for the equilibrium capacity
Qe	the numerical value for the adsorbed capacity

Value

the linear regression and the parameters for the Langmuir isotherm

Author(s)

Mark Lester Galicia

C.C. Deocaris

References

Langmuir, I. (1917). The constitution and fundamental properties of solids and liquids II. Liquids. Journal of American Chemistry Society, 1848-1906.

Liu, L., Luo, X.-B., LinDing, & Sheng-LianLuo. (2019). Application of Nanotechnology in the Removal of Heavy Metal From Water. Nanomaterials for the Removal of Pollutants and Resource Reutilization, 83-147.

Examples

```
Ce <- c(0.01353, 0.04648, 0.13239, 0.27714, 0.41600, 0.63607, 0.80435, 1.10327, 1.58223)
Qe <- c(0.03409, 0.06025, 0.10622, 0.12842, 0.15299, 0.15379, 0.15735, 0.15735, 0.16607)
langmuir.LM1(Ce, Qe)
```

---

langmuiranalysis *Langmuir Isotherm Analysis Non-Linear Form*

Description

The Langmuir adsorption isotherm is used to describe the equilibrium between adsorbate and adsorbent system, where the adsorbate adsorption is limited to one molecular layer at or before a relative pressure of unity is reached.

Usage

```
langmuiranalysis(Ce, Qe)
```

Arguments

Ce	the numerical value for the equilibrium capacity
Qe	the numerical value for the adsorbed capacity

Value

the linear regression and the parameters for the Langmuir isotherm

Author(s)

Mark Lester Galicia

C.C. Deocaris

References

Langmuir, I. (1997). The constitution and fundamental properties of solids and liquids II. Liquids. Journal of American Chemistry Society, 1848-1906.

Liu, L., Luo, X.-B., LinDing, & Sheng-LianLuo. (2019). Application of Nanotechnology in the Removal of Heavy Metal From Water. Nanomaterials for the Removal of Pollutants and Resource Reutilization, 83-147.

Examples

```
Ce <- c(0.01353, 0.04648, 0.13239, 0.27714, 0.41600, 0.63607, 0.80435, 1.10327, 1.58223)
Qe <- c(0.03409, 0.06025, 0.10622, 0.12842, 0.15299, 0.15379, 0.15735, 0.15735, 0.16607)
langmuiranalysis (Ce, Qe)
```

---

langmuirFanalysis *Langmuir-Freundlich Isotherm Analysis Non-Linear Form*

Description

Langmuir-Freundlich Isotherm Analysis describes the distribution of adsorption energy onto heterogeneous surfaces of the adsorbent. At low concentrations of adsorbate, this model becomes Freundlich isotherm, and then at high concentration of adsorbate, it becomes the Langmuir Isotherm. The parameters of this concentration can be obtained using the non-linear regression.

Usage

```
langmuirFanalysis(Ce, Qe)
```

Arguments

`Ce`	the numerical value for the equilibrium capacity
`Qe`	the numerical value for the adsorbed capacity

Value

the linear regression and the parameters for the Langmuir-Freundlich isotherm

Author(s)

Cabugnason, Jay Anne M.

Pogado, Precious Grace

C.C. Deocaris

References

Jeppu G.P and Clement T.P. (2012, March 15) A modified Langmuir-Freundlich isotherm model for simulating pH-dependent adsorption effects. Retrieved from: www.researchgate.net/publication/221762917_A_modified_La Freundlich_isotherm_model_for_simulating_pH-dependent_adsorption_effects

Umpleby R.J., et. al (2001, August 23) Characterization of Molecularly Imprinted Polymers with the Langmuir-Freundlich Isotherm. Retrieved fromhttps://pubs.acs.org/doi/pdf/10.1021/ac0105686

Examples

```
Ce <- c(0.06649, 0.21948, 0.38188, 0.56311, 0.77729, 0.98794, 1.25390, 1.72698)
Qe <- c(0.05192, 0.07174, 0.08680, 0.09433, 0.08839, 0.08363, 0.09711, 0.10741)
langmuirFanalysis(Ce, Qe)
```

---

mjanalysis *Marckzewski-Jaroniec Isotherm Analysis Non-Linear Form*

Description

The Marczewski-Jaroniec Isotherm model is the resemblance of Langmuir Isotherm model. It is developed on the basis of the supposition of local Langmuir isotherm and adsorption energies distribution in the active sites on adsorbent (Parker, 1995; Sivarajasekar & Baskar, 2014). This equation comprises all isotherm equations being an extension of simple Langmuir Isotherm to single solute adsorption on heterogeneous solids (Marczewski & Jaroniec, 1983).

Usage

```
mjanalysis(Ce, Qe)
```

Arguments

Ce	the numerical value for the equilibrium capacity
Qe	the numerical value for the absorbed capacity

Value

The non-linear regression and the parameters for Marckzewski Jaroniec Isotherm Analysis

Author(s)

Brent Mark A. Daniel

Charlestone E. Antatico

C.C. Deocaris

References

Marczewski, A.W., Jaroniec, M. (1983). A new isotherm equation for single-solute adsorption from dilute solutions on energetically heterogeneous solids. Monatsh Chem 114, 711-715. doi: 10.1007/BF01134184

Parker Jr, G.R. (1995). Optimum isotherm equation and thermodynamic interpretation for aqueous 1,1,2- trichloroethene adsorption isotherms on three adsorbents. Adsorption, 1 (2): 113-132. doi:10.1007/BF00705000

Sivarajasekar, N., Baskar, R. (2014). Adsorption of basic red 9 onto activated carbon derived from immature cotton seeds: Isotherm studies and error analysis. Desalination and Water Treatment, 52: 1-23. doi:10.1080/19443994.2013.834518

Examples

```
mjanalysis(moringa$Ce,moringa$Qe)
```

`moringa` *Moringa Adsorption Study*

Description

Actual adosrption experiment results using Moringa oleifera seeds.

Usage

```
moringa
```

Format

A data frame with 6 observations on the following 2 variables.

`Ce` a numeric vector

`Qe` a numeric vector

...

raudkepanalysis *Radke-Prausniiz Isotherm Analysis Nonlinear Form*

Description

Nonlinear form of the Radke-Prausniiz Equation, the original form. The Radke-Prausnitz isotherm model has several important properties which makes it more preferred in most adsorption systems at low adsorbate concentration.

Usage

```
raudkepanalysis(Ce, Qe)
```

Arguments

Ce	the numerical value for the equilibrium capacity
Qe	the numerical value for the adsorbed capacity

Value

the nonlinear regression and the parameters for the Raudke-Prausniiz isotherm

Author(s)

Princess Joyce DL Reyes

Neil Ross S. Alayon

C.C. Deocaris

References

Newton, A., & Donbebe. (2017, September 5). Modelling and Interpretation of Adsorption Isotherms. Retrieved from https://doi.org/10.1155/2017/3039817

Khalid, A., Kazmi, M. et.al, (2015). Kinetic & Equilibrium Modelling of Copper Biosorption. Retrieved from http://journals.pu.edu.pk/journals/index.php/jfet/article/view/527

Examples

```
raudkepanalysis(moringa$Ce,moringa$Qe)
```

`redlichpanalysis` *Redlich-Peterson Non-Linear Form*

Description

It is used for three parameter adsorption and its a combination of Langmuir and Freundlich Isotherms

Usage

```
redlichpanalysis(Ce, Qe)
```

Arguments

`Ce`	the numerical value for the equilibrium capacity
`Qe`	the numerical value for the adsorbed capacity

Value

the linear regression and the parameters for the Redlich-Peterson isotherm

Author(s)

John Carlo F. Panganiban

C.C. Deocaris

References

Ayawei, N., Ebelegi, A. N., & Wankasi, D. (2017). Modelling and Interpretation of Adsorption Isotherms. Journal of Chemistry, 2017, 1.11. doi: 10.1155/2017/3039817

Wu, F.-C., Liu, B.-L., Wu, K.-T., & Tseng, R.-L. (2010). A new linear form analysis of Redlich?Peterson isotherm equation for the adsorptions of dyes. Chemical Engineering Journal, 162(1), 21.27. doi: 10.1016/j.cej.2010.03.006

Examples

```
redlichpanalysis(moringa$Ce,moringa$Qe)
```

secondorder *Pseudo-2nd Order Kinetics*

Description

The pseudo-second order model describes the adsorption reaction rate with depndent energetically hetrogenousites on the adsorbent. (Mercado-Borayo, et. al., 2014)

Usage

```
secondorder(t, Ce)
```

Arguments

t	duration of the experiment
Ce	the numerical value for the equilibrium capacity

Value

the regression analysis for the second order kinetics

Examples

```
secondorder(c(1,2,3,4,5),c(1,2,3,4,5))
```

sipsanalysis *Sips Isotherm Analysis Non linear Form*

Description

This model is suitable for predicting adsorption on heterogeneous surfaces, thereby avoiding the limitation of increased adsorbate concentration normally associated with the Freundlich model.

Usage

```
sipsanalysis(Ce, Qe)
```

Arguments

Ce	the numerical value for the equilibrium capacity
Qe	the numerical value for the adsorbed capacity

Value

the nonlinear regression and the parameters for the Sips isotherm

References

N'diaye, A., Bollahi, M.,Kankou, M. (2019). Sorption of paracetamol from aqueous solution using groundnut shell as a low cost sorbent. J. Mater. Environ. Sci., 2019, Vol.10, Issue 6, 553-562.

Nethaji, S.,Sivasamy, A., Mandal, A. B. (2012). Adsorption isotherms, kinetics and mechanism for the adsorption of cationic and anionic dyes onto carbonaceous particles prepared from Juglans regia shell biomass. Int. J. Environ. Sci. Technol. (2013)10:231-242. doi: 10.1007/s13762-012-0112-0

Examples

```
sipsanalysis(moringa$Ce,moringa$Qe)
```

`summaryanalysis` *Summary of the Isotherm Analysis*

Description

1-2 sentences Summarize the analysis for different isotherm models

Usage

```
summaryanalysis(Ce, Qe)
```

Arguments

`Ce`	the numerical value for the equilibrium capacity
`Qe`	the numerical value for the adsorbed capacity

Value

summary of the nonlinear and linear fitting for different adsorption isotherm models

---

`temkinanalysis` *Temkin Isotherm Analysis Linear Form*

Description

takes into account the effects of indirect adsorbate/ adsorbate interaction on the adsorption process

Usage

```
temkinanalysis(Ce, Qe)
```

Arguments

`Ce`	wherein theta is is the numerical value for the equilibrium capacity
`Qe`	is Qe the numerical value for the adsorbed capacity

Value

the nonlinear regression and the parameters for the Flory-Huggins isotherm

Author(s)

Lance E. Abadier

C.C. Deocaris

References

Newton, A., & Donbebe. (2017, September 5). Modelling and Interpretation of Adsorption Isotherms. retrieved from: https://www.hindawi.com/journals/jchem/2017/3039817

Examples

```
Ce <- c(0.01353, 0.04648, 0.13239, 0.27714, 0.41600, 0.63607, 0.80435, 1.10327, 1.58223)
Qe <- c(0.03409, 0.06025, 0.10622, 0.12842, 0.15299, 0.15379, 0.15735, 0.15735, 0.16607)
temkinanalysis(Ce, Qe)
```

---

tothanalysis *Toth Isotherm Analysis Non-Linear Form*

Description

Another empirical modification of the Langmuir equation with the aim of reducing the error between experimental data and predicted value of equilibrium data.

Usage

```
tothanalysis(Ce, Qe)
```

Arguments

Ce	the numerical value for the equilibrium capacity
Qe	the numerical value for the fractional coverage

Value

The non linear regression and the parameters for the Toth isotherm analysis

Author(s)

Kim Zyrell P. Zagala

C.C. Deocaris

References

Gutierrez, L.G., et.al(2018, September 20), Kinetic and Equilibrium Study of the Absorption of CO2 in Ultramicropores of Resorcinol-Formaldehyde Aerogels obtained in Acidic and Basic Medium. Retrieved from: doi:10.3390/c4040052

Ayawei, N. (2017, September 05). Medelling an Interpretation of Adsorption Isotherm. Retrieved from: https://www.hidawi.com/journals/jchem/2017/3039817

Examples

```
tothanalysis(c(1,2,3,4,5),c(1,2,3,4,5))
```

`webervvanalysis` *Weber Van-Vliet Isotherm Analysis Non-linear Form*

Description

it provides an excellent description of data patterns for a broad range of systems. This model is suitable for batch rate and fixed-bed modelling procedures as it gives a direct parameter evaluation.

Usage

```
webervvanalysis(Qe, Ce)
```

Arguments

`Qe`	the numerical value for the adsorbed capacity
`Ce`	the numerical value for the equilibrium capacity

Value

the nonlinear regression and the parameters for Weber-Van-Vliet Isotherm Analysis

Author(s)

Jeann M. Bumatay

Leslie F. Bautista

Chester C. Deocaris

References

Van Vliet, B.M., Weber Jr., Hozumi, H.. (1979). Modeling and prediction of specific compound adsorption by activated carbon and synthetic adsorbents. Water Research Vol.14, pp. 1719 to 1728. https://doi.org/10.1016/0043-1354(80)90107-4

Examples

```
webervvanalysis(moringa$Qe,moringa$Ce)
```

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